Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for "An Accurate Benchmark Description of the Interactions between Carbon Dioxide and Polyheterocyclic Aromatic Compounds Containing Nitrogen"

Sicheng Li, Daniel G. A. Smith and Konrad Patkowski

*Department of Chemistry and Biochemistry, Auburn University, Auburn, AL*36849, *USA*

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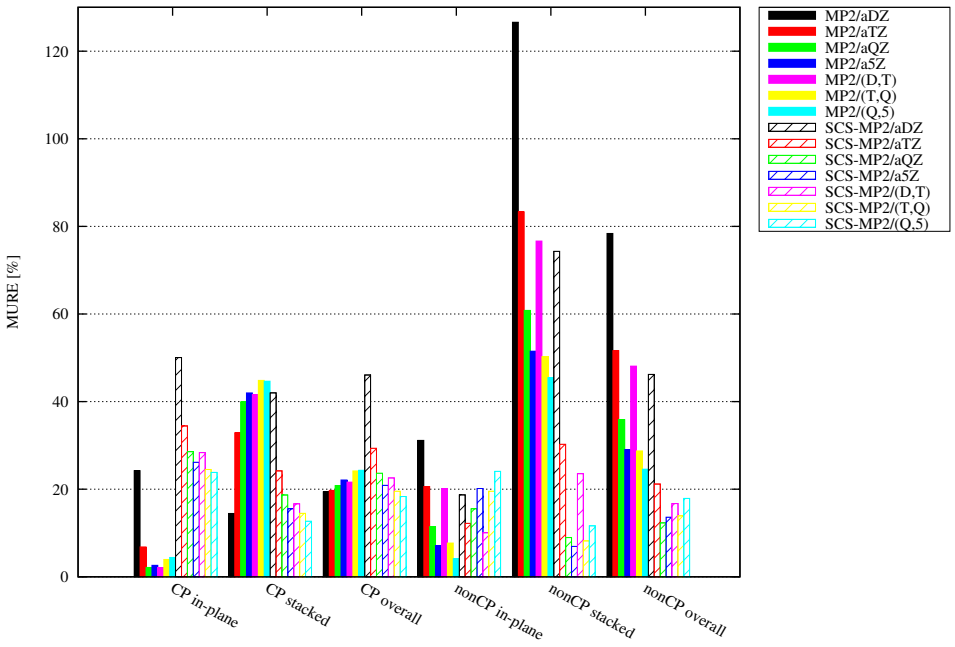

FIG. S1. The mean unsigned relative errors (MURE) for MP2 and SCS-MP2 compared, both CP-corrected and nonCP-corrected, to the CCSD(T)/CBS-level benchmark values as defined in the text. The "CP" means CP-corrected, and "nonCP" represents the nonCP-corrected values. The "overall" label signifies the results of all stacked and in-plane structures.

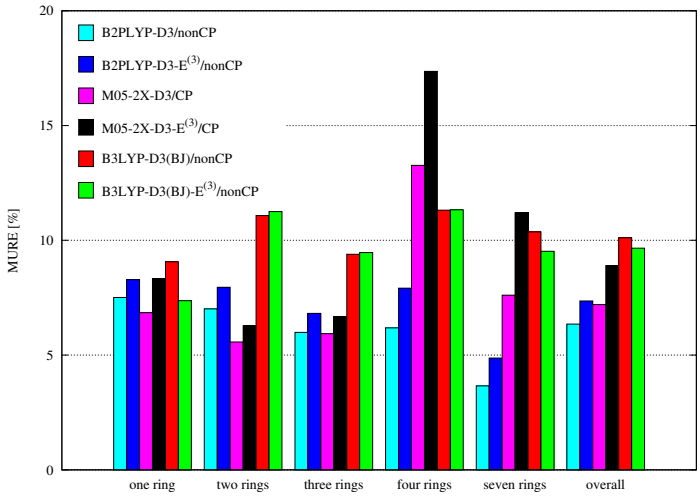

FIG. S2. The mean unsigned relative errors (MURE) for the best performers: M05-2X-D3/CP, M05-2X-D3-$E^{(3)}$/CP, B2PLYP-D3/nonCP, B2PLYP-D3-$E^{(3)}$/nonCP, B3LYP-D3(BJ), B3LYP-D3(BJ)-$E^{(3)}$/nonCP, in the largest basis set QZVP computed, as functions of the number of rings in the N-PHAC molecule (the overall MURE for all 95 N-PHAC-CO_2 geometries is displayed in the last column) against the MP2/CBS+ΔCCSD(T) benchmark interaction energies.

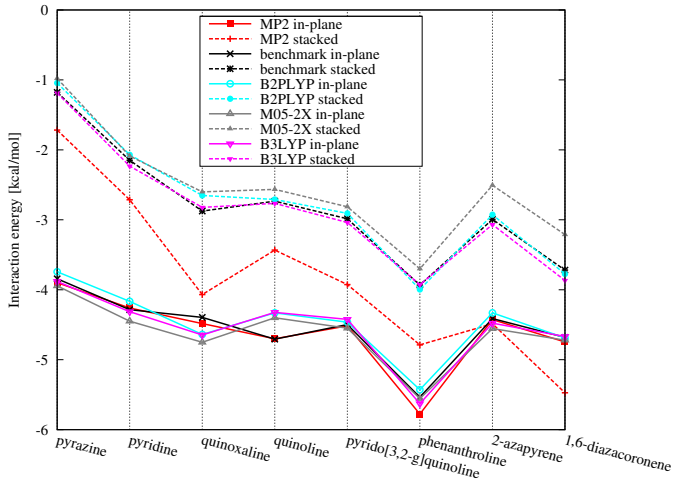

FIG. S3. Comparison of the interaction energies calculated by different approaches for the in-plane and stacked minimum structures (obtained as described in the text) of all N-PHAC-CO_2 dimers considered here. The MP2 values are taken from MP2-F12/(Q,5) for the seven symmetric 1- and 2-ring systems and MP2/(Q,5) for larger systems. The benchmark values are calculated at the MP2+ΔCCSD(T) level as described in the text. The DFT results are: B2PLYP-D3/$^{\mathrm{nonCP}}_{\mathrm{QZVP}}$, M05-2X-D3/$^{\mathrm{CP}}_{\mathrm{QZVP}}$, and B3LYP-D3(BJ)/$^{\mathrm{nonCP}}_{\mathrm{QZVP}}$.